Nanocrystals in the Manufacture of Target for Inertial Confinement Fusion.

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The efficiency of power generation in inertial confinement fusion is related, among other phenomena, to development in the manufacture of deuterium tritium target, in particular the solid layer of this material (DT ice). The requirements for the target manufacture are several, within the most salient this roughness and thickness variation of the solid layer [1], these are related to the hydrodynamic instabilities that occur at the time of compression, decreasing the efficiency ignition and burning of fuel, for example the Rayleigh-Taylor instability [2]. One of the ways to reduce these instabilities is the growth of nanocrystals in the solid layer of DT-ice, thus obtained solid structures more rigid and with a speed of sound propagation uniform [3]. In this work we present a simulation methodology [4] which is obtained by varying the speed of sound, to the solid structures of atomic isotopes of hydrogen in high pressure conditions. These simulations are performed for different grain sizes. The study is a first step in the analysis of the relationship between the growth of nanocrystals and ignition efficiency.

Systems inertial confinement fusion (ICF) need of a manufacturing process targets very accurate and efficient (Fig. A). Due to the frequency needed for energy production techniques are necessary to achieve high repetition rates, however it is also necessary to increase or maintain the quality and efficiency of these targets. In order to observe more resolution possible problems in the target manufacture (B), we propose the following theoretical methodology, by means of which analyze different phenomena present in the conditions which are fabrication and handled deuterium tritium target spheres (DT ice). Recent experiments show that addition of instabilities caused by the geometry of the solid layer of DT ice (C), and the cover (ablator), one can relate the loss of power delivery in the implosion due to different conformations of the solid layers with regarding handling conditions [5,6].

INSTABILITIES CAUSED BY (Fig. D):
1) Roughness
2) Thickness
3) Different phases (percentage of liquid- solid).
4) Different structural phases in the solid (FCC-HCP)
5) ATG: solid growth (nanostructures)

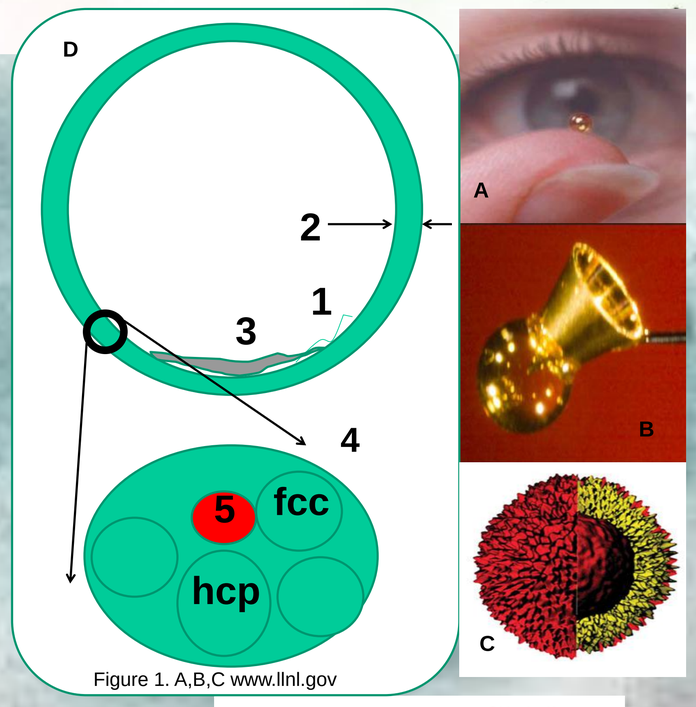
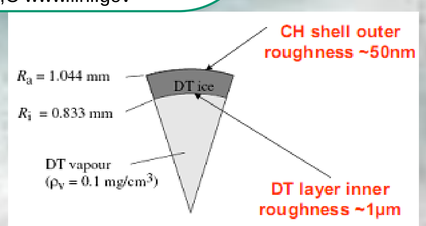


Figure 1. A,B,C www.llnl.gov

The solid layer and the hydrogen used as ablator foam (Beryllium, CH polymers, tantalum, etc.) have special characteristics (Fig. 2). One way to obtain these special conditions is to manufacture the solid layer with the growth of nanocrystals, this proposal is already being studied experimentally [7], and in this paper we propose a study using ab initio methods and molecular dynamics (MD), to know the mechanical properties of the nanostructured material.



Shell cross-section Figure 2. www.llnl.gov

Methodology

The process we use to model phase transitions, is the simulation using *ab initio* methods and Quantum Molecular Dynamics (QMD), through different codes in which we highlight SIESTA [8]. The process has 3 parts: A) defines a mixing H_2, D_2, T_2, HD, HT, DT, HDT you want to model, with a defined structure for the temperature to study. B) apply the energy minimization by two methods: the conjugate gradient (for 0 K) and QMD temperature, with Nose-Hoover thermostat only, C) finally with QMD Parrinello-Rahman barostat and N-H thermostat is set the temperature and pressure, increase or decrease in pressure is achieved by applying different ramps up or down [4]. Our initial structure around the all study is HCP as shown in Part A. The simulations is make with 600 atoms in PBC conditions [9].

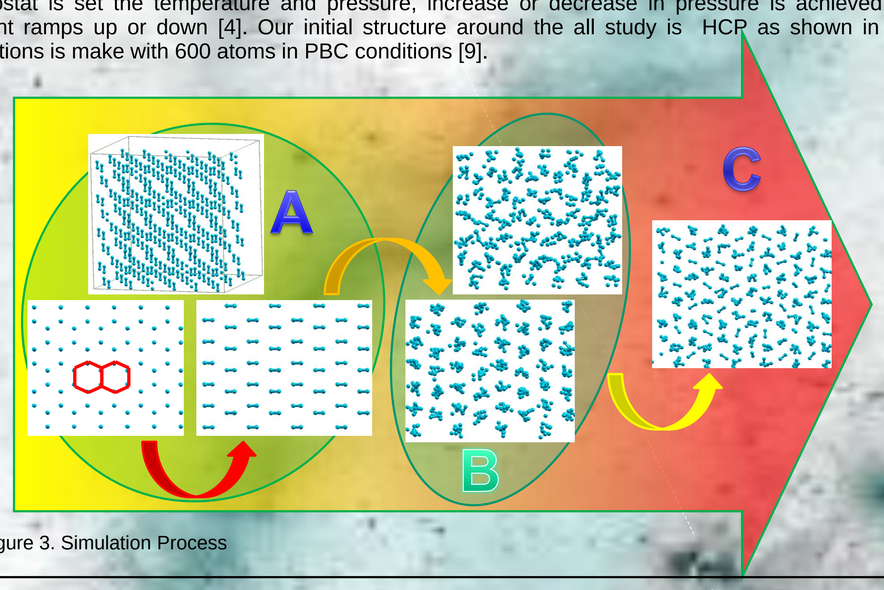


Figure 3. Simulation Process

High Pressure

In the range of high pressures our results show consistency with the phase diagrams between 1 GPa and 80 GPa [10,11], from a free rotor 1 GPa phase I, to restricted rotor 80 GPa phase II (Figure 4A). For pressures above 200 GPa the structure undergoes a phase transition above the phase III, from phase III to IV (not yet defined [12]). The crystalline configuration are hexagons distributed in planes (Figure 4B) that are close with increasing pressure, this phenomenon has been described by other authors [13]. These phases are not well described by the equations of state of hydrogen, much less for the DT ice, which should be well represented in the ICF model. The results shown are for 15 K, have also studied 300 K and 100 K.

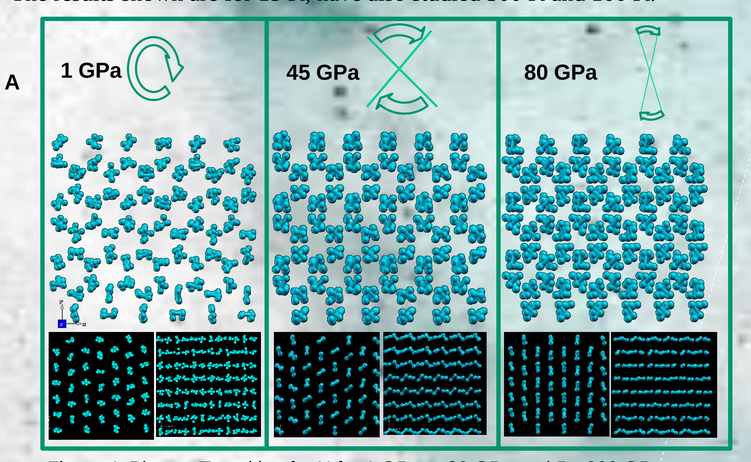
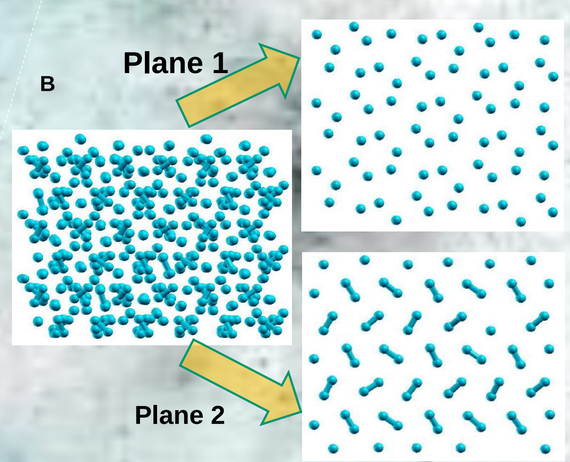
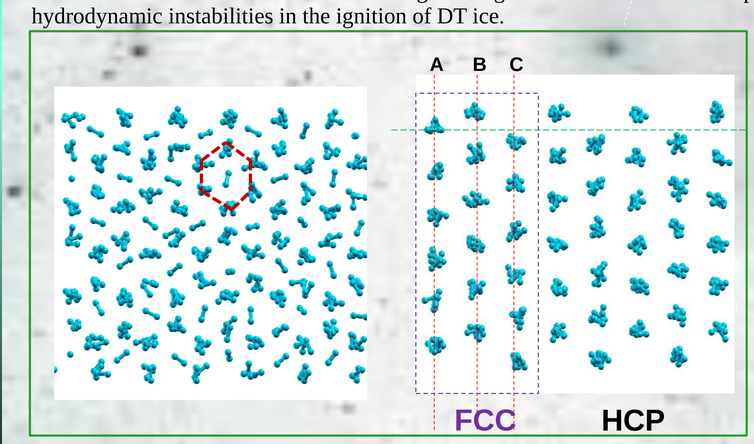


Figure 4. Phases Transition for H for 1 GPa to 80 GPa and P> 200 GPa.



Low Pressure

At pressures lower than 500 MPa, the results of the simulations show a phase transition, that is a mixture FCC and HCP. Such mixtures have been observed in experiments both near the triple point of hydrogen [14] and in DT ice [15]. Left in Figure 5 shows the results of the simulation, the initial system is a HCP crystal above 1 GPa, to down the pressure the crystal formed by a HCP-FCC mixture, the experimental Raman spectrum [14] for the same conditions shows the HCP-FCC mixture (Figure 5 right). Controlling the growth of these phases is of great interest in the manufacture and handling of targets in ICF. One of our purposes is to study the phase transition and relate possible hydrodynamic instabilities in the ignition of DT ice.



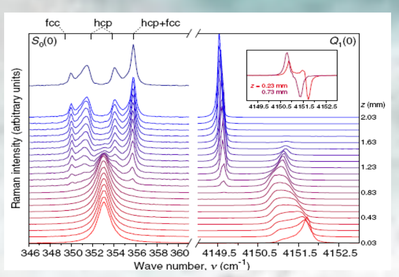


Figure 5. Phase Transition for low pressure (P< 500 MPa). Mix phase HCP-FCC theoretical results (left) and experimental Raman spectroscopy (right)

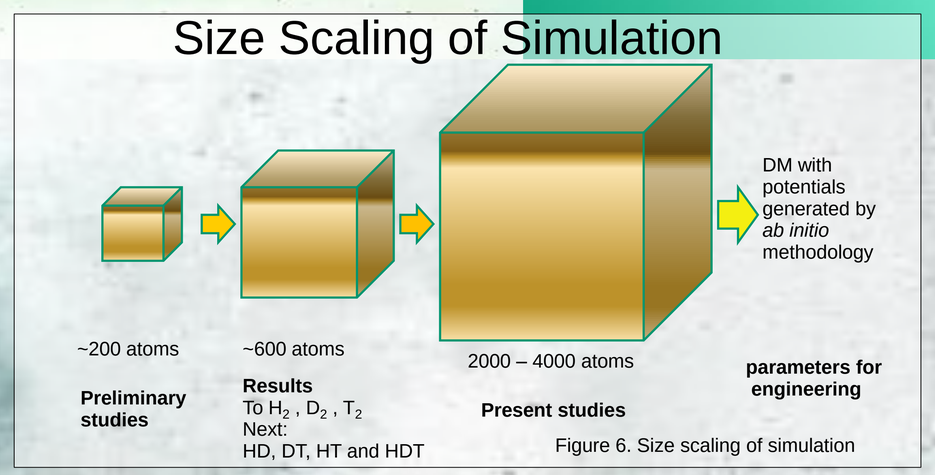


Figure 6. Size scaling of simulation

The results obtained so far are the first level of the multiscale methodology, this generated parameters from the simulations or first-principles calculations on scales of a few atoms (Figure 6), then increase the volume under study, through methods such as molecular dynamics and coming to representations of the continuous medium as finite element methods or generate the equations of state for hydrodynamic simulations.

Alekxandrova et al [7] discuss the way in which they must make the solid layer of DT ice, showing a difference between a regular solid and solid nanocrystalline grains of approximately ~ 20 nm (figure 7), although this is an approximation these studies have been improved by other groups in different materials. Bringa et al [3] studied the propagation of a wave in nanostructured copper, they show that the grain size affects the width of the wave, and sizes of nanoscopic grains (nanocrystals) help to ensure the reduction of fluctuations in the front wave, and to decrease the unwanted hydrodynamic instabilities.
The first step before working with nanocrystalline materials is to increase the volume of our crystal, from 600 to 4000 atoms (Figure 8), in order to observe the effects of size on phase changes already reported, at this point we have the cooperation CESVIMA of the UPM, and *Magerit* supercomputer with more than 4000 processors. The nanostructured solid molecular hydrogen is modeled using Molecular Dynamics and potential existing or partially generated by *ab initio* calculations (now we focus on this point)

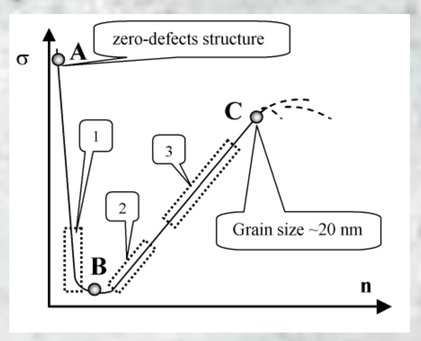
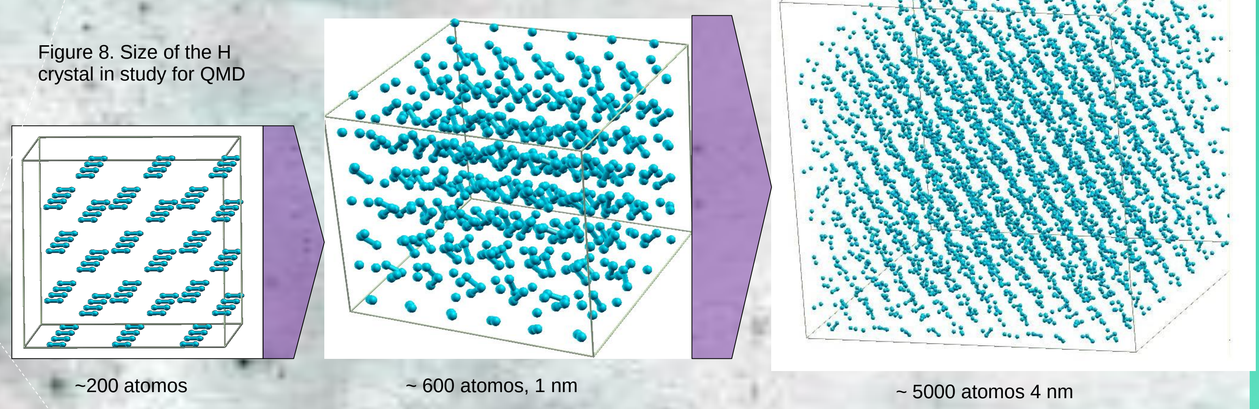


Figure 7. The graph shows a schematic approach of stiffness of a material vs.grain size. A single perfect crystal, (1) real crystal, (2) micrograin structure, (3) structure with ultra fine nanogranos [7]

Figure 8. Size of the H crystal in study for QMD



DT---ice Anisotropies And Nanocrystaline Structures In fuel pellets for IF targets.

Using *ab initio methods and advanced molecular dynamics we are predicting the properties of DT-ice* nanocrystaline structures in layers inside de fuel pellets. Influence over burning and pellet efficiency of this anisotropy is being evaluated via implosion hydrodynamics studies.
We seek to improve the characteristics of the solid layer to reduce the effects of instabilities and the sound velocity difference by means of a distribution of grain sizes determined (figure 9). This study will be extended to other materials in addition to solid hydrogen, such as beryllium, carbon (polymers) and tantalum.

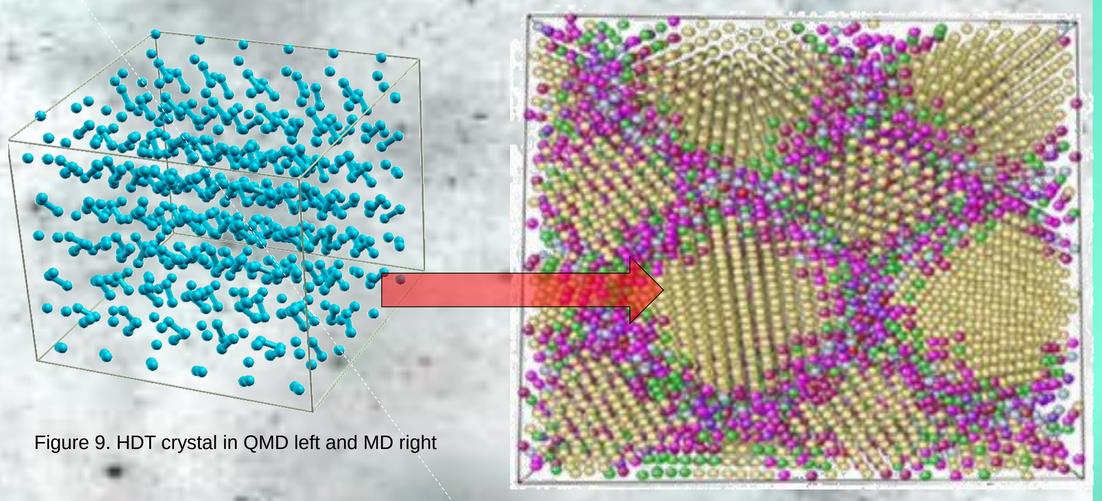


Figure 9. HDT crystal in QMD left and MD right

CONCLUSIONS

Have a simulation method whereby experimental results are reproduced. Phase transitions in high-pressure phase I and II [4] to 15 K we have found close to 50 GPa in parahydrogen [11]. With pressures greater than 200 GPa, hexagonal structures are observed in separate planes. We observed mixtures of HCP and FCC structures, in the range from 50 K to 100 K at pressures less than 500 MPa. This study has been extended to deuterium and tritium.
The speed of sound has discontinuities due to phase transitions, which must be studied with higher resolution.
We implemented a method by which to study possible changes in temperature and pressure points for phase transitions reported by us for different crystal volumes of hydrogen (besides DT ice)
As future work: Get theoretically Raman and IR spectrum near the triple point for mixtures of HD, DT, and for H_2 and D_2 (in collaboration with Laboratory of Molecular Fluid Dynamics, IEM-CSIC)[14]. Study materials at high pressure, especially carbon, iron and aluminum (with the support of high-pressure experimental group at the Complutense University of Madrid). Study of the interfaces between Dt ice and materials of the capsule as Beryllium, Carbon and Tantalum.

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Small steps lead to big leaps ... and the moon ... in memory Neil Armstrong